LETTERS TO NATURE

power-law dependence on the current, particularly if multiple inelastic scattering events are required. The observed sideways motion of the xenon atom at greater tip-sample separation is consistent with the xenon atom being vibrational excited. The absence of sideways motion at closer tip-sample separation may be due to the increased van der Waals attraction to the tip as the tip is brought closer to the surface. Heating-assisted electromigration is the only mechanism of which we are aware that is consistent with all the observed phenomena.

Note that the atom switches we have constructed are macroscopic devices in the sense that most of the power dissipation occurs not in the atomic-scale volume of the active element but in a volume comparable to the cube of the inelastic mean free path of electrons in the terminals of the switch. Furthermore, our macroscopic terminals do not show the quantum size effects that atomic-scale leads would exhibit.

It is clear that serious obstacles lie between what we have demonstrated and the realization of a genuinely useful atomic-scale device.\footnote{1} The prospect of atomic-scale logic and memory devices is nonetheless a little closer. We are intrigued by the idea that atom switches might already exist in the form of single cage-like molecules which derive their switching function from an atom that is trapped in the cage.

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Electronic states and phases of $K_xC_{60}$ from photoemission and X-ray absorption spectroscopy


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HIGH-resolution photoemission and soft X-ray absorption spectroscopies have provided valuable information on the electronic structure near the Fermi energy in the superconducting copper oxide compounds,\footnote{1-4} helping to constrain the possible mechanisms of superconductivity. Here we describe the application of these techniques to $K_xC_{60}$, found recently to be superconducting below 19.3 K for $x \approx 3$ (ref. 5). The photoemission and absorption spectra as a function of $x$ can be fitted by a linear combination of data from just three phases, $C_{60}$, $K_3C_{60}$ and $K_6C_{60}^*$, indicating that there is phase separation in our samples. The photoemission spectra clearly show a well defined Fermi edge in the $K_3C_{60}$ phase with a density of states of $5.2 \times 10^3$ electrons eV$^{-1}$ Å$^{-3}$ and an occupied-band width of 1.2 eV, suggesting that this phase may be a weakly coupled BCS-like (conventional) superconductor. The C1s absorption spectra show large non-rigid-band shifts between the three phases with half and complete filling, in the $K_3C_{60}$ and $K_6C_{60}$ phases respectively, of the conduction band formed from the lowest unoccupied molecular orbital of $C_{60}$. These observations clearly demonstrate that the conduction band has $C_{2p}$ character. The non-rigid-band shift coupled with the anomalous occupied-band width implies that there is significant mixing of the electronic states of $K$ and $C_{60}$ in the superconducting phase.

A mixture of fullerenes was synthesized by contact arc evaporation\footnote{8} of graphite under 300 torr of He. After Soxhlet extraction with toluene, $C_{60}$ was separated from the mixture by column chromatography on neutral alumina with 5% toluene in hexane as eluant. The purity of $C_{60}$ was 99.9% relative to $C_{70}$ impurity. The sample was bulk-dried under vacuum for several hours at 200°C, then heated in flowing $N_2$ to 325°C before use. Pure $C_{60}$ (ref. 8) was evaporated from a pyrex ampule in an ultrahigh-vacuum chamber and potassium was obtained from a SAES getter source. Both sources were outgassed for several hours after the system was baked. $C_{60}$ was deposited onto a clean Cu(100) substrate at room temperature until a film of thickness $\geq 200$ Å was obtained. Potassium was evaporated onto the carbon film which was subsequently annealed at 100°C for ~1 h. After the sample had returned to room temperature, the photoemission and absorption spectra were recorded. The concentration of potassium was controlled by sequential evaporation and annealing steps until a saturated $K_3C_{60}$ sample was obtained. All spectra were measured using the AT&T Bell Laboratories Dragon high-resolution soft X-ray beam line at the National Synchrotron Light Source\footnote{9,10}, with the experimental resolution set at 120 meV for photoemission spectra, 60 meV for absorption spectra.

Figure 1 shows a set of photoemission spectra of the valence-band region of $K_xC_{60}$ as a function of $x$. The bottom curve is for pure $C_{60}$, which is nearly identical to the spectrum published by Weaver et al.\footnote{11} The second curve labelled $x = 0.5$ has basically the same features as the pure $C_{60}$ spectrum, except that the small concentration of $K$ has created a Fermi edge 2.6 eV above the highest occupied molecular orbital (HOMO) peak of $C_{60}$. The third curve labelled $x = 1$ has the same features as the pure $C_{60}$ spectrum, except that the small concentration of $K$ has created a Fermi edge 2.6 eV above the highest occupied molecular orbital (HOMO) peak of $C_{60}$. As the $K$ concentration is increased by sequential evaporation and annealing, the valence-band spectra can be seen to change. The most marked change is the clear

![Binding energy (eV)](https://example.com/binding-energy.png)

**FIG. 1** Valence-band photoemission spectra of $K_xC_{60}$ as a function of $x$. The Fermi edge region has been enlarged (×3) with the background subtracted. Energy $h\nu = 110$ eV. 603

NATURE . VOL 352 . 15 AUGUST 1991
development of a Fermi edge; that is, the sample becomes metallic. The region near the Fermi energy ($E_F$) shows that the sample starts as an insulator, becomes a metal with a maximum intensity of the excitation to the LUMO of C60 decreases while the intensity of the K 2p → 3d absorption (near $h\nu = 297$ eV) increases.

Two previous reports of the photoemission spectra of K$_x$C$_{60}$ have been published, but neither of these investigations shows the clear development of the Fermi level intensity as seen in Fig. 1. No soft X-ray absorption spectra have been reported for K$_x$C$_{60}$.

The K concentration was determined in three ways: using the intensity of the peak near $E_F$ in Fig. 1, the intensity of the K absorption in Fig. 2 and a fitting procedure applied to the valence-band structure of K$_x$C$_{60}$.

The data presented in Fig. 1 for the valence-band structure near $E_F$ indicate that there are only three phases: C$_{60}$ with no structure within ~2 eV of $E_F$, K$_3$C$_{60}$ with a filled band ~0.6 eV below $E_F$, and K$_6$C$_{60}$ with a filled band ~0.6 eV below $E_F$. Figure 3 shows this region of the spectra for these three phases. The curve for K$_3$C$_{60}$ was generated from the $\tilde{x} = 3.1$ curve by removing a small contribution from the saturated spectrum. The DOS at $E_F$ can be directly measured from the spectral intensity at $E_F$ after the instrumental broadening has been removed. The conversion of the intensity scale to states per electronvolt per K$_3$C$_{60}$ molecule is accomplished by using the HOMO of the K$_3$C$_{60}$ as a reference. This band is derived from the LUMO of C$_{60}$ which contains three states (six electrons). An alternative normalization using the area of the conduction band itself gives almost identical results. Our measured DOS at $E_F$ is $1.9 = \pm 0.1$ states per eV per K$_3$C$_{60}$, equivalent to $5.2 \times 10^{-3}$ electrons eV$^{-1}$ Å$^{-2}$. To extract the occupied-band width of the conduction band of K$_3$C$_{60}$, the data are fitted with a free-electron-like (FE) band, $N(\epsilon) = N(\epsilon_F^0)/\left[1 + (\epsilon - \epsilon_F^0)/\epsilon_F^0\right]^{1/2}$, convoluted with a gaussian instrumental response function (solid line). The occupied-band width is found to be 1.2 ± 0.05 eV. As this band is derived from the C 2p atomic orbitals, a tight-binding-like (TB) band has also been used to fit the data. The standard deviation of the TB fit (not shown) is twice times larger than that of the FE fit, but gives a similar occupied-band width. This occupied-band width in K$_3$C$_{60}$ is almost the same as the full-band width of the HOMO in K$_6$C$_{60}$. In weak-coupling BCS theory, the transition temperature is related to the DOS by the relationship $T_c = 1.13 E_\text{p} \exp[ -1/(N(\epsilon_F)^{1/2})]$, where $E_\text{p}$ is the energy of the pairing-mediation excitation, $\alpha_{\text{p}}$ is the electron-excitation coupling strength and $\lambda = N(\epsilon_F)$ is the coupling constant. Cheng and Klein15 have calculated the phonon modes for both the face-centred cubic and body-centred cubic phases of K$_3$C$_{60}$, observing that the low-energy translational and librational motions of the C$_{60}$ molecules are strongly coupled to the K motion. If we use the energy of 30 cm$^{-1}$ found for the face-centred cubic phase, we obtain a value of $\lambda = 1.06$, which is large for weak coupling. This value of $\lambda$ is due to the low frequency of the coupled librational-translational modes and should be considered as an upper limit. Even for this $\lambda$ we have $\alpha_{\text{p}} = 0.56$ eV, corresponding to a deformation potential $\alpha_{\text{p}} = 0.27$ eV Å$^{-1}$. This is a relatively modest matrix element for electron-phonon scattering, consistent with K$_3$C$_{60}$ being a BCS superconductor.

The original X-ray diffraction studies of K$_x$C$_{60}$ powders indicated that for $0 < x < 6$ the sample was almost completely phase-separated into C$_{60}$ and K$_6$C$_{60}$ (ref. 18), consistent with the first report of superconductivity in K$_x$C$_{60}$, where it was claimed that only 1% of the sample contributed to the superconducting phase. Recently, Holzner et al.16 showed that there was a single superconducting phase K$_x$C$_{60}$, which is now believed to be face-centred cubic with K incorporated into all of the octahedral and tetrahedral interstices. All of the spectral features near $E_F$ in Fig. 1 can be fitted with the three pure-phase spectra shown in Fig. 3. It is slightly more difficult to fit the absorption spectra in a similar fashion, because the three phases have markedly different structures. The absorption spectrum for pure K$_3$C$_{60}$ was constructed from the difference between the spectrum for $\tilde{x} = 0.9$ and the pure C$_{60}$ spectrum from the difference between the last two curves in the doping sequence. The assumption was that if there is phase separation, as indicated by the

FIG. 3 Photoemission spectra near the Fermi edge for three phases of K$_x$C$_{60}$ ($hv = 110$ eV).
LETTERS TO NATURE

Magnetic-field penetration depth in \( K_3C_{60} \) measured by muon spin relaxation


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The discovery of superconductivity in \( C_{60} \) doped with the alkali metals potassium and rubidium has introduced a new family of three-dimensional molecular superconductors. The potassium-doped compound \( K_3C_{60} \) has a relatively high transition temperature \( T_c = 19.3 \) K, a very high upper critical field \( H_{c2}(T \to 0) = 50 T \) and a short superconducting coherence length \( \xi = 26 \) \( \AA \), in common with the copper oxide superconductors. Here we report muon-spin-relaxation measurements of the magnetic-field penetration depth \( \lambda \) in \( K_3C_{60} \). The temperature dependence of \( \lambda \) and of the muon spin relaxation rate indicate that the superconducting energy gap is isotropic, without nodes or zero points. The low-temperature penetration depth \( \lambda(T \to 0) \) is about 4,800 \( \AA \), which implies a ratio of superconducting carrier density to effective mass to be \( \rho/(m^*m_c) = 1.2 \times 10^{10} \) cm\(^{-2}\) if one assumes the 'clean limit'. Combining this result with the value of \( \xi \), we estimate the Fermi temperature \( T_F = 470 \) K. In the relationship between \( T_F \) and \( T_c \), \( K_3C_{60} \) conforms to the trend exhibited by 'exotic' superconductors \(^{1,2} \), such as the Chevrel phase compounds, the copper oxides and the organic BEDT-TTF systems.

The muon-spin-relaxation (\( \mu \)-SR) technique has been extensively applied in the study of the penetration depth in various type-II superconductors. \(^{3-5} \) In transverse-field \( \mu \)-SR (TF-\( \mu \)-SR) measurements of \( \lambda \), we apply an external magnetic field \( H_{ext} \) \( (H_{ext} \ll H_{c1} \ll H_{c2}) \), and observe the spin precession of positive muons implanted in the specimen. In the superconducting state, the field \( H_{ext} \) forms a lattice of flux vortices in the specimen, resulting in a local magnetic field \( B \) having a distribution with a width \( \Delta B \) proportional to \( \lambda^{-2} \). In the spectra of muon spin precession, the oscillation amplitudes are damped because of the inhomogeneity of the local field. This damping is usually described by a gaussian envelope \( G(t) = \exp \left( -\alpha t^2 \right) \), which defines the muon spin relaxation rate \( \alpha = \Delta B \lambda^{-2} \).

The specimen of \( K_3C_{60} \) was prepared at UCLA following the procedures described in ref. 3. A polycrystalline powder material weighing 135 mg was pressed into a sintered pellet ~1 cm in diameter and 1 mm thick. Before pressing, the powder sample showed a shielding diamagnetism ranging from 40 to 60% of a bulk niobium reference. The difference from the reference is mostly due to the small packing density of the powder. Pressing and sintering results in an onset of bulk (100%) shielding at a temperature \( \sim 1 \) K lower than \( T_c = 19.3 \) K (ref. 11). X-ray studies on a similar specimen \(^6 \), sensitive to microscopic-scale inhomogeneity, set an upper limit of 15% volume fraction for presumably nonsuperconducting minority phases. The sintered specimen for \( \mu \)-SR was mounted in a \( \text{He} \) gas flow cryostat with its face normal to the beam direction along which the external field was applied. During the whole procedure of sample preparation and \( \mu \)-SR measurements, the specimen was kept under vacuum or in dry \( \text{He} \) gas, except for an interval of less than 1